Molecular-Scale Structure, Modeling and Thermodynamic Properties of Aqueous Nickel Chloride Solutions at High Temperatures

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Molecular-level insight into the physical and chemical properties of solutions can be attained through the combination of detailed information on the structure of aqueous electrolyte solutions with accurate thermodynamic measurements. Enthalpies of dilution were measured at temperatures from 323 to 523 K, with solutions acidified to prevent hydrolysis of nickel at elevated temperatures. Analysis of the molality dependence of the dilution enthalpies indicates minimal ion association in solution under experimental conditions; temperature integration of the results gives activity coefficients for aqueous nickel chloride over the full temperature range studied. Using neutron diffraction with isotopic substitution (NDIS), the hydration structure of aqueous nickel chloride solutions has been determined over a range of temperatures. These experiments probe the structure near the aqueous nickel ion, with emphasis on the structure of the first solvation shell. Further insight into hydration and complexation in solution has been obtained through our recent molecular-dynamics simulations of the structure and properties of nickel chloride solutions, focusing on an understanding of the detailed atomic-level interactions giving rise to observed structural and thermodynamic features. Results of this experimental and modeling work will be described, with emphasis on the fuller picture of solution properties obtained from the combination of structural, thermodynamic, and modeling studies.